

# Non-Markovian quantum state diffusion for an open quantum system in fermionic environments

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Non-Markovian quantum state diffusion (NMQSD) provides a powerful approach to the dynamics of an open quantum system in bosonic environments. Here we develop an NMQSD method to study the open quantum system in fermionic environments. This was a long-standing problem involving anticommutative noise functions (i.e., Grassmann variables) that are intrinsically different from the noise functions of bosonic baths. We obtain the NMQSD equation for quantum states of the system and the non-Markovian master equation. Moreover, we apply this NMQSD method to single and double quantum-dot systems.

*Introduction.*— The theory of open quantum systems has become an increasingly important topic in, e.g., quantum information science, quantum measurement, and quantum optics. Traditionally, the dynamics of an open quantum system was often investigated using a Markov master equation derived by invoking the Born-Markov approximation. However, this formalism fails for many solid-state systems (see, e.g., [1]) where the system-environment coupling is strong and the environment is structured. Thus a non-Markovian master equation is required when considering the memory effect and back action of the environment. It is known that the derivation of an exact non-Markovian master equation has long been a challenging task. One of the breakthroughs is the exact non-Markovian master equation for quantum Brown motion model derived by Hu *et al.* [2] using the Feynman-Vernon influence functional path-integral method [3].

Of all the theoretical strategies used to deal with open quantum systems, a non-Markovian quantum trajectory theory known as non-Markovian quantum state diffusion (NMQSD) [4, 5] provides a powerful approach to the dynamics of an open quantum system in bosonic environments. In this approach, when the so-called  $O$ -operator is obtained, the quantum dynamics of an open system is determined by solving the NMQSD equation (i.e., a diffusive stochastic Schrödinger equation) and the non-Markovian master equation can also be derived [6, 7]. In contrast to the conventional master equation under the Born approximation, this non-Markovian master equation is derived non-perturbatively, so it applies even for a strong system-environment coupling. Indeed, some exact  $O$ -operators have been found in a variety of quantum models [4–9], including multilevel models [10].

In addition to bosonic baths, fermionic baths are also involved in many physical systems, particularly in solid-state systems. The Feynman-Vernon influence functional path-integral method can also be used to study the quantum dynamics of an open system in a fermionic environment (see, e.g., [11]). Recently, this path-integral method was extended to derive the non-Markovian master equation

of a double-quantum-dot system [12]. Nevertheless, the extension of NMQSD method to an open quantum system in fermionic baths has been a long-standing unsolved problem because this open system involves anticommutative noise functions (i.e., Grassmann variables) that are intrinsically different from the noise functions of bosonic baths. In this Letter, we develop an NMQSD method to study the open quantum system in fermionic baths. This NMQSD approach is formulated in a non-perturbative manner and it applies for both weak and strong system-environment couplings. We not only obtain the NMQSD equation for quantum states of the system, but also derive the non-Markovian master equation. Moreover, as interesting examples, we apply this NMQSD method to single and double quantum-dot systems.

*Quantum state diffusion equation.*—We consider a quantum system coupled to two fermionic baths:  $H = H_{\text{sys}} + H_{\text{env}} + H_{\text{int}}$ , with (we set  $\hbar = 1$ )

$$H_{\text{env}} = \sum_k (\omega_{Lk} a_{Lk}^\dagger a_{Lk} + \omega_{Rk} a_{Rk}^\dagger a_{Rk}), \quad (1)$$

$$H_{\text{int}} = \sum_k (g_{Lk} c_L^\dagger a_{Lk} + g_{Rk} c_R^\dagger a_{Rk} + \text{H.c.}). \quad (2)$$

Here  $H_{\text{sys}}$  denotes the Hamiltonian of the system,  $H_{\text{env}}$  is the Hamiltonian of the two electric leads acting as fermionic baths, and  $H_{\text{int}}$  models the interactions between the system and the two baths. The spectral density function of each bath is  $J_\lambda(\omega) = \sum_k |g_{\lambda k}|^2 \delta(\omega - \omega_{\lambda k})$ , where  $\lambda = L$  or  $R$ . In Eq. (1),  $a_{\lambda k}^\dagger$  ( $a_{\lambda k}$ ) is the fermionic creation (annihilation) operator for a quantum state with wave vector  $k$  in the left or right lead. We assume that the system of interest couples to the two leads via single channels characterized by the fermionic creation (annihilation) operators  $c_{\lambda k}^\dagger$  ( $c_{\lambda k}$ ) [see Eq. (2)]. Extension to a multi-channel case is straightforward.

In an NMQSD approach, environments are required to be initially at zero temperature, so as to conveniently represent the environmental degrees of freedom with the coherent state basis. As for environments initially

with a nonzero temperature, one can map the nonzero-temperature density operator to a zero-temperature density operator using a Bogoliubov transformation [13]. In the case of fermionic baths, this requires to add  $\sum_{\lambda k} \omega_{\lambda k} b_{\lambda k} b_{\lambda k}^\dagger$  to Eq. (1), corresponding to the part involving holes in the electric leads. The Bogoliubov transformation for fermionic operators can be introduced as

$$\begin{aligned} a_{\lambda k} &= \sqrt{1 - \bar{n}_{\lambda k}} d_{\lambda k} - \sqrt{\bar{n}_{\lambda k}} e_{\lambda k}^\dagger \\ b_{\lambda k} &= \sqrt{1 - \bar{n}_{\lambda k}} e_{\lambda k} + \sqrt{\bar{n}_{\lambda k}} d_{\lambda k}^\dagger, \end{aligned} \quad (3)$$

where  $\bar{n}_{\lambda k} = [e^{(\omega_{\lambda k} - \mu_\lambda)/k_B T} + 1]^{-1}$  is the average number of electrons in the  $k$ th state of the left (right) electric lead with chemical potential  $\mu_\lambda$ . In Eq. (3), the coefficients are determined by the requirement that the derived master equation reduces to a Lindblad form in the Markovian limit. The transformed Hamiltonian  $\mathcal{H}$  is written as

$$\begin{aligned} \mathcal{H} &= H_{\text{sys}} + \sum_{\lambda k} \left[ \omega_{\lambda k} (d_{\lambda k}^\dagger d_{\lambda k} + e_{\lambda k} e_{\lambda k}^\dagger) \right. \\ &\quad \left. + (\sqrt{\bar{n}_{\lambda k}} g_{\lambda k}^* c_\lambda e_{\lambda k} + \sqrt{1 - \bar{n}_{\lambda k}} g_{\lambda k} c_\lambda^\dagger d_{\lambda k} + \text{H.c.}) \right], \end{aligned} \quad (4)$$

where the new fermionic operator  $d_{\lambda k}$  ( $e_{\lambda k}^\dagger$ ) corresponds to the annihilation of electrons (holes) in the virtual fermionic baths. Note that the effects of temperature are incorporated into the transformed Hamiltonian and the fermionic baths with *nonzero* initial temperatures are mapped to virtual fermionic baths with *zero* initial temperature.

In the interaction picture with respect to the environmental Hamiltonian  $\mathcal{H}_{\text{env}} = \sum_{\lambda k} \omega_{\lambda k} (d_{\lambda k}^\dagger d_{\lambda k} + e_{\lambda k} e_{\lambda k}^\dagger)$ , the total Hamiltonian reads

$$\begin{aligned} \mathcal{H}(t) &= H_{\text{sys}} + \sum_{\lambda k} (\sqrt{\bar{n}_{\lambda k}} g_{\lambda k}^* c_\lambda e_{\lambda k} e^{i\omega_{\lambda k} t} \\ &\quad + \sqrt{1 - \bar{n}_{\lambda k}} g_{\lambda k} c_\lambda^\dagger d_{\lambda k} e^{-i\omega_{\lambda k} t} + \text{H.c.}), \end{aligned} \quad (5)$$

and the quantum state of the total system satisfies the equation of motion

$$\partial_t |\Psi_t\rangle = -i\mathcal{H}(t) |\Psi_t\rangle. \quad (6)$$

We assume that the quantum state of the total system is factorized at the initial time  $t = 0$ , so that  $|\Psi_0\rangle = |\varphi_0\rangle \otimes |0\rangle$ , with the virtual fermionic baths initially in the ground state (i.e., at zero temperature):  $|0\rangle = \bigotimes_{\lambda} |0\rangle_{\lambda d} \otimes |0\rangle_{\lambda e}$ , where  $d_{\lambda k}|0\rangle = 0$ , and  $e_{\lambda k}|0\rangle = 0$ .

Define a fermionic coherent-state basis for the environmental degrees of freedom:  $|zw\rangle = \bigotimes_{\lambda} |z\rangle_{\lambda} \otimes |w\rangle_{\lambda}$ , with

$$\begin{aligned} |z\rangle_{\lambda} &= \bigotimes_k |z_k\rangle_{\lambda} = e^{-\sum_k z_{\lambda k} d_{\lambda k}^\dagger} |0\rangle \\ |w\rangle_{\lambda} &= \bigotimes_k |w_k\rangle_{\lambda} = e^{-\sum_k w_{\lambda k} e_{\lambda k}^\dagger} |0\rangle, \end{aligned} \quad (7)$$

where  $z_k$  and  $w_k$  are Grassmann variables that obey the anticommutation relation. With the completeness relation for coherent states  $\int e^{-z^* z - w^* w} |zw\rangle \langle zw| d^2 z d^2 w =$

1, the state  $|\Psi_t\rangle$  can be expressed as

$$|\Psi_t\rangle = \int e^{-z^* z - w^* w} |zw\rangle \otimes |\psi_t(z^*, w^*)\rangle d^2 z d^2 w, \quad (8)$$

where  $z^* z \equiv \sum_{\lambda k} z_{\lambda k}^* z_{\lambda k}$ ,  $w^* w \equiv \sum_{\lambda k} w_{\lambda k}^* w_{\lambda k}$ ,  $d^2 z \equiv \prod_{\lambda k} dz_{\lambda k}^* dz_{\lambda k}$ , and  $d^2 w \equiv \prod_{\lambda k} dw_{\lambda k}^* dw_{\lambda k}$ . The actions of annihilation (creation) operators  $d_{\lambda k}$  and  $e_{\lambda k}$  ( $d_{\lambda k}^\dagger$  and  $e_{\lambda k}^\dagger$ ) on fermionic coherent states satisfy the relations [14]:  $d_{\lambda k}|z\rangle_{\lambda} = z_{\lambda k}|z\rangle_{\lambda}$ ,  $d_{\lambda k}^\dagger|z\rangle_{\lambda} = -\frac{\partial}{\partial z_{\lambda k}}|z\rangle_{\lambda}$ ,  $e_{\lambda k}|w\rangle_{\lambda} = w_{\lambda k}|w\rangle_{\lambda}$ , and  $e_{\lambda k}^\dagger|w\rangle_{\lambda} = -\frac{\partial}{\partial w_{\lambda k}}|w\rangle_{\lambda}$ . When projecting onto the coherent-state basis, the equation of motion (6) can be reduced to the NMQSD equation for a pure state of the system  $|\psi_t(z^*, w^*)\rangle \equiv \langle zw|\Psi_t\rangle$ :

$$\begin{aligned} \frac{\partial}{\partial t} |\psi_t\rangle &= -iH_{\text{sys}} |\psi_t\rangle - \sum_{\lambda} \left[ c_{\lambda} z_{\lambda}^*(t) |\psi_t\rangle + c_{\lambda}^\dagger w_{\lambda}^*(t) |\psi_t\rangle \right] \\ &\quad - \sum_{\lambda} c_{\lambda}^\dagger \int_0^t \alpha_{\lambda 1}(t-s) \frac{\delta}{\delta z_{\lambda}^*(s)} |\psi_t\rangle ds \\ &\quad - \sum_{\lambda} c_{\lambda} \int_0^t \alpha_{\lambda 2}(t-s) \frac{\delta}{\delta w_{\lambda}^*(s)} |\psi_t\rangle ds, \end{aligned} \quad (9)$$

which initiates from  $|\psi_{t=0}(z^*, w^*)\rangle = |\varphi_0\rangle$ . Here the noise functions  $z_{\lambda}^*(t)$  and  $w_{\lambda}^*(t)$  are defined as

$$\begin{aligned} z_{\lambda}^*(t) &= -i \sum_k \sqrt{1 - \bar{n}_{\lambda k}(\omega_{\lambda k})} g_{\lambda k}^* z_{\lambda k}^* e^{i\omega_{\lambda k} t}, \\ w_{\lambda}^*(t) &= -i \sum_k \sqrt{\bar{n}_{\lambda k}(\omega_{\lambda k})} g_{\lambda k} w_{\lambda k}^* e^{-i\omega_{\lambda k} t}. \end{aligned} \quad (10)$$

The temperature-dependent environment correlation functions are  $\alpha_{\lambda 1}(t-s) \equiv \mathcal{M}\{z_{\lambda}(t) z_{\lambda}^*(s)\} = \int dw [1 - \bar{n}_{\lambda}(w)] J_{\lambda}(w) e^{-i\omega(t-s)}$ , and  $\alpha_{\lambda 2}(t-s) \equiv \mathcal{M}\{w_{\lambda}(t) w_{\lambda}^*(s)\} = \int dw \bar{n}_{\lambda}(w) J_{\lambda}(w) e^{i\omega(t-s)}$ , where  $\mathcal{M}\{\cdot\}$  denotes the statistical mean over all noise variables:  $\mathcal{M}\{\cdot\} \equiv \int e^{-z^* z - w^* w} \{\cdot\} d^2 z d^2 w$ .

Introducing  $O$ -operators by  $\frac{\delta}{\delta z_{\lambda}^*(s)} |\psi_t(z^*, w^*)\rangle = O_{\lambda 1}(t, s, z^*, w^*) |\psi_t(z^*, w^*)\rangle$ , and  $\frac{\delta}{\delta w_{\lambda}^*(s)} |\psi_t(z^*, w^*)\rangle = O_{\lambda 2}(t, s, z^*, w^*) |\psi_t(z^*, w^*)\rangle$ , we can write the NMQSD equation in a time-local form:

$$\begin{aligned} \frac{\partial}{\partial t} |\psi_t\rangle &= -iH_{\text{sys}} |\psi_t\rangle - \sum_{\lambda} \left[ c_{\lambda} z_{\lambda}^*(t) + c_{\lambda}^\dagger w_{\lambda}^*(t) \right. \\ &\quad \left. + c_{\lambda}^\dagger \bar{O}_{\lambda 1}(t, z^*, w^*) + c_{\lambda} \bar{O}_{\lambda 2}(t, z^*, w^*) \right] |\psi_t\rangle, \end{aligned} \quad (11)$$

where  $\bar{O}_{\lambda n} \equiv \int_0^t ds \alpha_{\lambda n}(t-s) O_{\lambda n}(t, s, z^*, w^*)$ ,  $n = 1, 2$ .

With the consistency conditions  $\frac{\partial}{\partial t} \frac{\delta |\psi_t\rangle}{\delta z_{\lambda}^*(s)} = \frac{\delta}{\delta z_{\lambda}^*(s)} \frac{\partial |\psi_t\rangle}{\partial t}$  and  $\frac{\partial}{\partial t} \frac{\delta |\psi_t\rangle}{\delta w_{\lambda}^*(s)} = \frac{\delta}{\delta w_{\lambda}^*(s)} \frac{\partial |\psi_t\rangle}{\partial t}$ , as well as the initial conditions  $O_{\lambda 1}(t, s, z^*, w^*)|_{t=s} = c_{\lambda}$  and  $O_{\lambda 2}(t, s, z^*, w^*)|_{t=s} = c_{\lambda}^\dagger$ , we obtain the equations of motion for the  $O$ -

operators:

$$\begin{aligned} \frac{\partial O_{\lambda n}}{\partial t} = & [-iH_{\text{sys}} - \sum_{\lambda'} (c_{\lambda'}^\dagger \bar{O}_{\lambda'1} + c_{\lambda'} \bar{O}_{\lambda'2}), O_{\lambda n}] + Q_n \\ & + \sum_{\lambda'} \left( \{c_{\lambda'}, O_{\lambda n}\} z_{\lambda'}^*(t) + \{c_{\lambda'}^\dagger, O_{\lambda n}\} w_{\lambda'}^*(t) \right), \end{aligned} \quad (12)$$

where the square and curly brackets denote the commutator and anticommutator, respectively, and  $Q_n = c_L^\dagger \frac{\delta \bar{O}_{L1}}{\delta \Lambda_n} + c_R^\dagger \frac{\delta \bar{O}_{R1}}{\delta \Lambda_n} + c_L \frac{\delta \bar{O}_{L2}}{\delta \Lambda_n} + c_R \frac{\delta \bar{O}_{R2}}{\delta \Lambda_n}$ , with  $\Lambda_1 = z_\lambda^*(s)$  and  $\Lambda_2 = w_\lambda^*(s)$ .

*Master equation.*—The reduced density operator of an open quantum system by tracing over the environmental degrees of freedom can be obtained by taking the statistical mean on a density operator related to the state  $|\psi_t(z^*, w^*)\rangle$ :

$$\rho_t = \text{Tr}_{\text{env}} |\Psi_t\rangle \langle \Psi_t| = \mathcal{M}\{P_t\}, \quad (13)$$

where  $P_t \equiv |\psi_t(z^*, w^*)\rangle \langle \psi_t(-z, -w)|$ . Using the relation  $\frac{\partial P_t}{\partial t} = \frac{\partial |\psi_t(z^*, w^*)\rangle \langle \psi_t(-z, -w)|}{\partial t} + |\psi_t(z^*, w^*)\rangle \frac{\partial \langle \psi_t(-z, -w)|}{\partial t}$  and Eq. (11), we derive the following non-Markovian master equation:

$$\begin{aligned} \frac{\partial \rho_t}{\partial t} = & -i[H_{\text{sys}}, \rho_t] + \sum_{\lambda} \left( [c_\lambda, \mathcal{M}\{P_t \bar{O}_{\lambda 1}^\dagger(t, -z, -w)\}] \right. \\ & - [c_\lambda^\dagger, \mathcal{M}\{\bar{O}_{\lambda 1}(t, z^*, w^*) P_t\}] \\ & - [c_\lambda, \mathcal{M}\{\bar{O}_{\lambda 2}(t, z^*, w^*) P_t\}] \\ & \left. + [c_\lambda^\dagger, \mathcal{M}\{P_t \bar{O}_{\lambda 2}^\dagger(t, -z, -w)\}] \right). \end{aligned} \quad (14)$$

This master equation is derived non-perturbatively, so it applies even for a strong coupling between the system and the environments. Moreover, in addition to trace preserving, it also preserves the positivity and hermiticity.

In the Markovian limit,  $\alpha_{\lambda 1}(t-s) \rightarrow [1 - \bar{n}_\lambda] \Gamma_\lambda \delta(t-s)$ , and  $\alpha_{\lambda 2}(t-s) \rightarrow \bar{n}_\lambda \Gamma_\lambda \delta(t-s)$ , where  $\Gamma_\lambda = 2\pi \rho_\lambda |g_\lambda|^2$ , with  $\lambda = L (R)$ , is the electron tunneling rate between the system and the left (right) lead. Also, the time-integrated  $O$ -operators become  $\bar{O}_{\lambda 1} \rightarrow \frac{1}{2} \Gamma_\lambda (1 - \bar{n}_\lambda) c_\lambda$ , and  $\bar{O}_{\lambda 2} \rightarrow \frac{1}{2} \Gamma_\lambda \bar{n}_\lambda c_\lambda^\dagger$ . Therefore, the master equation (14) is reduced to

$$\begin{aligned} \frac{\partial \rho_t}{\partial t} = & -i[H_{\text{sys}}, \rho_t] \\ & + \sum_{\lambda} \frac{\Gamma_\lambda}{2} \left[ \bar{n}_\lambda (2c_\lambda^\dagger \rho_t c_\lambda - c_\lambda c_\lambda^\dagger \rho_t - \rho_t c_\lambda c_\lambda^\dagger) \right. \\ & \left. + (1 - \bar{n}_\lambda) (2c_\lambda \rho_t c_\lambda^\dagger - c_\lambda^\dagger c_\lambda \rho_t - \rho_t c_\lambda^\dagger c_\lambda) \right]. \end{aligned} \quad (15)$$

It is clear that this Markov master equation has a Lindblad form.

*Application to quantum-dot systems.*—Below we apply our NMQSD approach to single and double quantum-dot systems.

(i) *Single quantum dot.* Suppose that the single quantum dot is in the strong Coulomb blockade regime, so that only one electron is allowed therein. The Hamiltonian of the system is written as  $H_{\text{sys}} = \omega_0 c^\dagger c$ , and  $c_L = c_R = c$  for  $H_{\text{int}}$  in Eq. (2). The non-Markovian master equation is exactly derived as

$$\begin{aligned} \frac{\partial \rho_t}{\partial t} = & -i[H_{\text{sys}}, \rho_t] + \Gamma_1(t) [c, \rho_t c^\dagger] + \Gamma_2(t) [c, c^\dagger \rho_t] \\ & - \Gamma_1^*(t) [c^\dagger, c \rho_t] - \Gamma_2^*(t) [c^\dagger, \rho_t c], \end{aligned} \quad (16)$$

with time-dependent rates

$$\Gamma_j(t) = \int_0^t [\alpha_1(s-t) A_j(t, s) - \alpha_2(t-s) B_j(t, s)] ds, \quad (17)$$

where  $\alpha_j(t) = \alpha_{Lj}(t) + \alpha_{Rj}(t)$ ;  $A_j(t, s)$  and  $B_j(t, s)$  are determined by the integro-differential equations:

$$\begin{aligned} \left( \frac{\partial}{\partial s} - i\omega_0 \right) A_j(t, s) + \int_0^s \beta(s-s') A_j(t, s') ds' &= U(t, s) \\ \left( \frac{\partial}{\partial s} - i\omega_0 \right) B_j(t, s) + \int_0^s \beta(s-s') B_j(t, s') ds' &= V(t, s), \end{aligned} \quad (18)$$

with  $\beta(s-s') \equiv \alpha_1(s'-s) + \alpha_2(s-s')$ ,  $U(t, s) \equiv \int_0^t \alpha_2(s-s') h(t, s') ds'$ ,  $V(t, s) \equiv \int_0^t \alpha_1(s'-s) h(t, s') ds'$ , and the final conditions at  $s = t$ :  $A_1(t, t) = B_1(t, t) = 1$ , and  $A_2(t, t) = B_2(t, t) = 0$ . Here  $h(t, s)$  satisfies the equation  $(\frac{\partial}{\partial s} - i\omega_0) h(t, s) - \int_s^t \beta(s-s') h(t, s') ds' = 0$ , with the final condition  $h(t, t) = 1$ .

In the Markovian limit,  $\Gamma_1(t) \rightarrow \frac{1}{2} [1 - \bar{n}_L(\omega_0)] \Gamma_L + \frac{1}{2} [1 - \bar{n}_R(\omega_0)] \Gamma_R$ , and  $\Gamma_2(t) \rightarrow -\frac{1}{2} \bar{n}_L(\omega_0) \Gamma_L - \frac{1}{2} \bar{n}_R(\omega_0) \Gamma_R$ . Let us consider the zero-temperature case with  $\bar{n}_\lambda(\omega_0) \rightarrow \theta(\mu_\lambda - \omega_0)$ , where  $\theta$  is the Heaviside step function. If the single-dot level  $\omega_0$  lies within the energy window  $\mu_L > \omega_0 > \mu_R$ , the master equation (16) reduces to  $\frac{\partial \rho_t}{\partial t} = -i\omega_0 [c^\dagger c, \rho_t] + \frac{1}{2} \Gamma_L (2c^\dagger \rho_t c - c c^\dagger \rho_t - \rho_t c c^\dagger) + \frac{1}{2} \Gamma_R (2c \rho_t c^\dagger - c^\dagger c \rho_t - \rho_t c^\dagger c)$ . With the basis state  $|0\rangle$  ( $|1\rangle$ ) which denotes an empty (occupied) dot, it follows that the density matrix elements satisfy

$$\begin{aligned} \dot{\rho}_{00} &= -\Gamma_L \rho_{00} + \Gamma_R \rho_{11}, \\ \dot{\rho}_{11} &= \Gamma_L \rho_{00} - \Gamma_R \rho_{11}, \\ \dot{\rho}_{10} &= -(i\omega_0 + \Gamma_L + \Gamma_R) \rho_{10}, \end{aligned} \quad (19)$$

which are exactly the rate equations obtained by Gurvitz and Prager [15].

(ii) *Double quantum dot (DQD).* Suppose that the DQD is in the strong Coulomb blockade regime, so that at most one electron is allowed in each dot. The Hamiltonian of the DQD can be written as  $H_{\text{sys}} = \omega_1 c_1^\dagger c_1 + \omega_2 c_2^\dagger c_2 + \Omega_0 (c_2^\dagger c_1 + c_1^\dagger c_2)$ , where  $\Omega_0$  denotes the inderdot coupling. For  $H_{\text{int}}$  in Eq. (2),  $c_L = c_1$ , and  $c_R = c_2$ . The exact non-Markovian master equation is given by

$$\begin{aligned}
\frac{\partial \rho_t}{\partial t} = & -i[H_{\text{sys}}, \rho_t] + \Gamma_{L1}(t)[c_1, \rho_t c_1^\dagger] + \Gamma_{L2}(t)[c_1, c_1^\dagger \rho_t] + \Gamma_{L3}(t)[c_1, \rho_t c_2^\dagger] + \Gamma_{L4}(t)[c_1, c_2^\dagger \rho_t] \\
& + \Gamma_{R1}(t)[c_2, \rho_t c_1^\dagger] + \Gamma_{R2}(t)[c_2, c_1^\dagger \rho_t] + \Gamma_{R3}(t)[c_2, \rho_t c_2^\dagger] + \Gamma_{R4}(t)[c_2, c_2^\dagger \rho_t] \\
& - \Gamma_{L1}^*(t)[c_1^\dagger, c_1 \rho_t] - \Gamma_{L2}^*(t)[c_1^\dagger, \rho_t c_1] - \Gamma_{L3}^*(t)[c_1^\dagger, c_2 \rho_t] - \Gamma_{L4}^*(t)[c_1^\dagger, \rho_t c_2] \\
& - \Gamma_{R1}^*(t)[c_2^\dagger, c_1 \rho_t] - \Gamma_{R2}^*(t)[c_2^\dagger, \rho_t c_1] - \Gamma_{R3}^*(t)[c_2^\dagger, c_2 \rho_t] - \Gamma_{R4}^*(t)[c_2^\dagger, \rho_t c_2],
\end{aligned} \tag{20}$$

with time-dependent coefficients

$$\Gamma_{\lambda j}(t) = \int_0^t [\alpha_{\lambda 1}(s-t)A_{\lambda j}(t,s) - \alpha_{\lambda 2}(t-s)B_{\lambda j}(t,s)]ds, \tag{21}$$

where  $A_{\lambda j}(t,s)$  and  $B_{\lambda j}(t,s)$  satisfy a set of integro-differential equations [16], with the final conditions:  $A_{L1}(t,t) = A_{R3}(t,t) = B_{L2}(t,t) = B_{R4}(t,t) = 1$ , and  $A_{\lambda j}(t,t) = 0$ ,  $B_{\lambda j}(t,t) = 0$  for other  $\lambda$  and  $j$ . A similar non-Markovian master equation was also obtained using the Feynman-Vernon influence functional path-integral method [12].

In the Markovian limit,  $\Gamma_{L1}(t) \rightarrow \frac{1}{2}[1 - \bar{n}_L(\omega_1)]\Gamma_L$ ,  $\Gamma_{R1} \rightarrow 0$ ;  $\Gamma_{L2}(t) \rightarrow -\frac{1}{2}\bar{n}_L(\omega_1)\Gamma_L$ ,  $\Gamma_{R2} \rightarrow 0$ ;  $\Gamma_{L3}(t) \rightarrow 0$ ,  $\Gamma_{R3} \rightarrow \frac{1}{2}[1 - \bar{n}_R(\omega_2)]\Gamma_R$ ; and  $\Gamma_{L4}(t) \rightarrow 0$ ,  $\Gamma_{R4} \rightarrow -\frac{1}{2}\bar{n}_R(\omega_2)\Gamma_R$ . We also consider the zero-temperature case with  $\bar{n}_\lambda(\omega_n) \rightarrow \theta(\mu_\lambda - \omega_n)$ , and the two single-dot levels of the DQD all lie within the energy window  $\mu_L > \omega_n > \mu_R$ , where  $n = 1, 2$ . We use  $|l\rangle$ ,  $l = 0, 1, 2$  and  $3$ , to denote the states with both dots empty, the left dot occupied, the right dot occupied, and both dots occupied, respectively. From Eq. (20), it follows that the master equations for density matrix elements are reduced to

$$\begin{aligned}
\dot{\rho}_{00} &= -\Gamma_L \rho_{00} + \Gamma_R \rho_{22}, \quad \dot{\rho}_{33} = \Gamma_L \rho_{22} - \Gamma_R \rho_{33}, \\
\dot{\rho}_{11} &= \Gamma_L \rho_{00} + \Gamma_R \rho_{33} + i\Omega_0(\rho_{12} - \rho_{21}), \\
\dot{\rho}_{22} &= -(\Gamma_L + \Gamma_R)\rho_{22} - i\Omega_0(\rho_{12} - \rho_{21}), \\
\dot{\rho}_{12} &= -i(\omega_1 - \omega_2)\rho_{12} + i\Omega_0(\rho_{11} - \rho_{22}) - \frac{\Gamma_L + \Gamma_R}{2}\rho_{12},
\end{aligned} \tag{22}$$

which are identical to the rate equations obtained in [12, 15]. For a DQD, both intradot and interdot Coulomb repulsions can play an important role in the Coulomb-blockade effect (see, e.g., [17]). Thus, if both intradot and interdot Coulomb repulsions are so strong that only one electron is allowed in the whole DQD, the master equations for density matrix elements are reduced to

$$\begin{aligned}
\dot{\rho}_{00} &= -\Gamma_L \rho_{00} + \Gamma_R \rho_{22} \\
\dot{\rho}_{11} &= \Gamma_L \rho_{00} + i\Omega_0(\rho_{12} - \rho_{21}) \\
\dot{\rho}_{22} &= -\Gamma_R \rho_{22} - i\Omega_0(\rho_{12} - \rho_{21}) \\
\dot{\rho}_{12} &= -i(\omega_1 - \omega_2)\rho_{12} + i\Omega_0(\rho_{11} - \rho_{22}) - \frac{\Gamma_R}{2}\rho_{12},
\end{aligned} \tag{23}$$

which are exactly the rate equations obtained in [18].

*Conclusion.*—We have developed an NMQSD method to study the dynamics of an open quantum system in fermionic baths. We not only obtain the NMQSD equation for quantum states of the system, but also derive the non-Markovian master equation. This non-Markovian approach is formulated in a non-perturbative manner and it applies even for a strong coupling between the system and the fermionic baths. Moreover, as useful examples, we have applied this NMQSD method to single and double quantum-dot systems.

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